Commensurate and Incommensurate Structure of the Neutron Cross Section in LaSrCu and YBaCuO

Ying-Jer Kao [a] ,Qimiao Si [b] , and K. Levin [a]

[a]James Franck Institute, The University of Chicago, 5640 South Ellis Avenue, Chicago, Illinois 60637

[b]Department of Physics, Rice University, Houston, TX 77251

We study the evolution of the d-wave neutron cross-section with variable frequency ω and fixed T (below and above T_c) in two different cuprate families. The evolution from incommensurate to commensurate to incommensurate peaks is rather generic within an RPA-like scheme. This behavior seems to be in reasonable accord with experiments, and may help distinguish between this and the "stripe" scenario.

The goal of the present paper is to address the frequency evolution of the neutron cross section, over the entire range of $\omega, \mathbf{q}$, using a scheme which we have previously applied to the normal[1] and d-wave superconducting states[2,3]. This work is viewed as significant because it leads to a fairly generic frequency evolution, which seems to be observed experimentally in two cuprate families[4–7]. These calculations, which have no adjustable parameters (besides those which were used to fit the normal state), can help establish whether the details of the fermiology plus d-wave pairing can account for the observed incommensurabilities and their evolution with frequency, or whether (by default) some new phenomenon such as stripe [8] or other exotic[9] phases may be required.

Our starting point is a three band, large U calculation[1] which yields a dynamical susceptibility $\chi(q,\omega) = \chi^o(q,\omega)/[1 + J(q)\chi^o(q,\omega)]$ where the Lindhard function χ^o is appropriate to the (d-wave) superconducting state and the underlying Fermi surface[2,10–12]. Here the residual exchange $J(q) = J_o[\cos q_x + \cos q_y]$ arises from Cu-Cu interactions via the mediating oxygen band. While the YBaCuO system is a two layer material, our past experience has shown that most of the peak structures associated with the neutron cross section are captured by an effective one layer band calculation, which we will investigate here. For definiteness, we fix the temperature at 4 K and vary frequency in increments of a few meV. We take the electronic excitation gap to be described by an ideal d-wave, $\Delta(q) = \Delta(\cos q_x + \cos q_y)$, where at $T = 4$ K, Δ is taken to be 17 meV in $YBaCuO_{6.6}$ and 8 meV in optimally doped LaSrCuO.

In Figure 1a we show the frequency evolution of an $YBaCuO_{6.6}$ sample. A node-to-node peak appears at low frequencies but the magnitude is small compared to that of all of the other features shown. Incommensurate peaks at $(\pi, \pi \pm \delta), (\pi \pm \delta, \pi)$ are first seen at around $\omega \approx \Delta$, albeit their magnitude is somewhat smaller than found experimentally. As frequency increases there is a clear trend: the incommensurability decreases continuously; this decrease is most apparent, in the immediate vicinity of the resonance frequency. At 27 meV the resonant, commensurate peak is now well established. As can be seen, there is some fine structure near (π, π) which is a remanent of the incommensurate peaks. And there is a pronounced evolution in the peak shape and height above resonance in the underdoped YBaCuO sample. The (π, π) regime is a flat-topped, possibly weakly incommensurate peak, just after resonance. It then broadens and remains structureless (as shown by our 34 meV plot) between $34 - 48$ meV. Finally, above 48 meV, clear incommensurate structure appears.

Figure 1b shows the frequency evolution for the LaSrCuO family, here shown at optimal doping. Node-to-node structures are seen at low frequencies with very small amplitude. A four peaked structure is seen at frequencies just around the gap frequency, 8 meV. These peaks are sharper, but in roughly the same position as their counterparts in the normal state[1]. These peaks persist (with slightly growing amplitude) until around 12 meV, at which point the incommen-

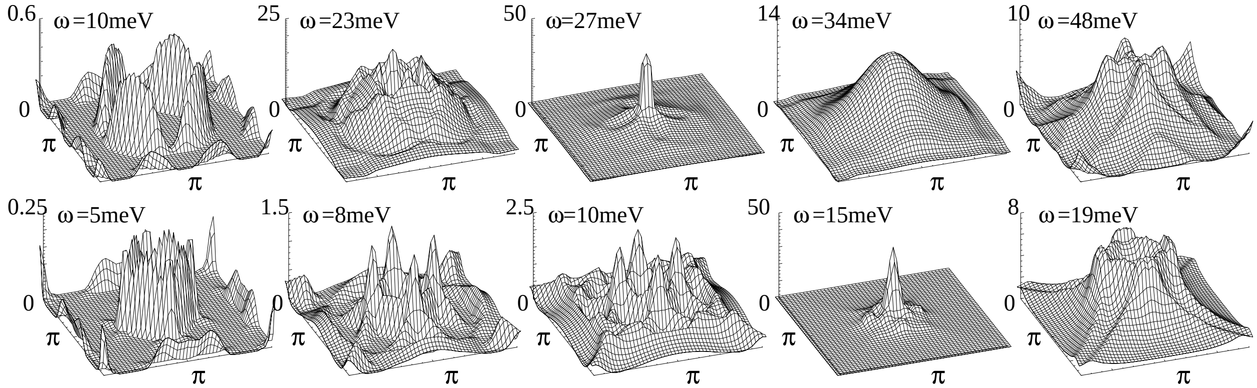

Figure 1. Frequency evolution of neutron cross section ($Im\chi$) for $YBaCuO_{6.6}$ (upper panel) and for optimal LaSrCuO (lower panel).

surability seems to decrease while their overall magnitude increases. In between 14 meV and $2\Delta = 16$ meV is an interesting (evidently "resonant") structure, but there have been, thus far, no reports of this resonance. However, it should be stressed, that if there is a commensurate feature in LaSrCuO, it should be seen only over a very narrow (≈ 2 meV) frequency window. Finally, just beyond 2Δ, as shown by the last panel at $\omega = 19$ meV, the cross section becomes very similar in shape to its normal state counterpart, although the magnitude is larger.

This evolution from incommensurate to commensurate peaks and then back to incommensurate behavior with increasing ω can, thus, be seen to be the case for both cuprates. There are claims for these effects in recent experiments on YBaCuO[6] and possibly in BiSSCO[5]. What appears to be different between our observations and these particular experiments[6] is that we do not find distinct two energy scales E_c, where the incommensurate peaks merge and E_r, where the resonance occurs. Our calculations for the reduced YBaCuO case, suggest that the incommensurate peaks probably never merge, but rather that at resonance the (π, π) feature fills in the gap between the two incommensurate features. In this sense E_c and E_r are the same frequency, although it should be stressed that here we have incorporated no resolution limiting effects.

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